



UNIVERSITI SAINS MALAYSIA

Final Examination  
2015/2016 Academic Session

May/June 2016

**JIK 227 – Chemical Spectroscopy**  
**[Spektroskopi Kimia]**

Duration : 3 hours  
[Masa : 3 jam]

Please ensure that this examination paper contains **TWENTY NINE** printed pages and an **Appendix** before you begin the examination.

Answer **FIVE** questions. Answer the questions in English. You may also answer the questions in Bahasa Malaysia, but not a mix of both languages.

All answers must be written in the answer booklet provided.

Each question is worth 20 marks and the mark for each sub question is given at the end of that question.

In the event of any discrepancies in the exam questions, the English version shall be used.

*Sila pastikan bahawa kertas peperiksaan ini mengandungi **DUA PULUH SEMBILAN** muka surat dan **Lampiran** yang bercetak sebelum anda memulakan peperiksaan ini.*

*Jawab **LIMA** soalan. Jawab soalan-soalan dalam Bahasa Inggeris. Anda juga dibenarkan menjawab soalan dalam Bahasa Malaysia, tetapi campuran antara kedua-dua bahasa ini tidak dibenarkan.*

*Setiap jawapan mesti dijawab di dalam buku jawapan yang disediakan.*

*Setiap soalan bernilai 20 markah dan markah subsoalan diperlihatkan di penghujung subsoalan itu.*

*Sekiranya terdapat sebarang percanggahan pada soalan peperiksaan, versi Bahasa Inggeris hendaklah diguna pakai.*

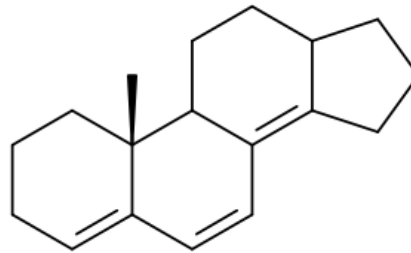
Answer **FIVE** (5) Question.

Jawab **LIMA** (5) Soalan.

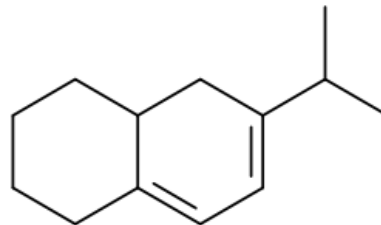
1. (a) Calculate  $\lambda_{max}$  for the compounds below.

*Kira  $\lambda_{max}$  bagi sebatian di bawah.*

(i)



(ii)



(6 marks/markah)

- (b) The absorbance of an iron thiocyanate solution containing 0.005 mg/mL was reported as 0.49 at 540 nm.

*Nilai serapan bagi larutan besi tiosianat yang mengandungi 0.005 mg/mL dilaporkan sebanyak 0.49 pada 540 nm.*

- (i) What is the molar absorptivity of iron thiocyanate on the assumption that a 1.00-cm cuvette was used?

*Apakah keserapan molar bagi besi tiosianat dengan beranggapan bahawa suatu kuvet 1.00-cm telah digunakan?*

- (ii) What will be the absorbance if the solution is diluted to twice its original volume?

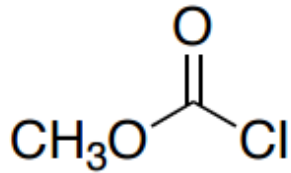
*Apakah nilai serapan jika larutan tersebut dicairkan sebanyak dua kali daripada isipadu asal?*

(4 marks/markah)

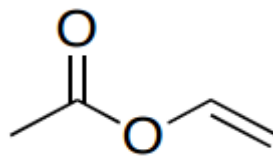
- 3 -

- (c) Each of the following IR spectra is associated with one of the compounds below. Identify the compound associated with each spectrum.

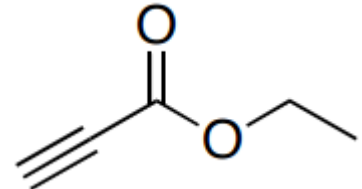
*Setiap spektrum IR berikut adalah berkaitan dengan satu daripada sebatian di bawah. Kenalpasti sebatian yang berkaitan dengan setiap spektrum.*



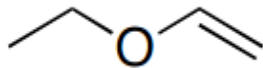
methyl chloroformate



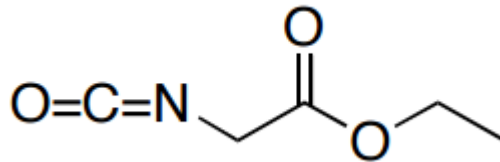
vinyl acetate



ethyl propiolate

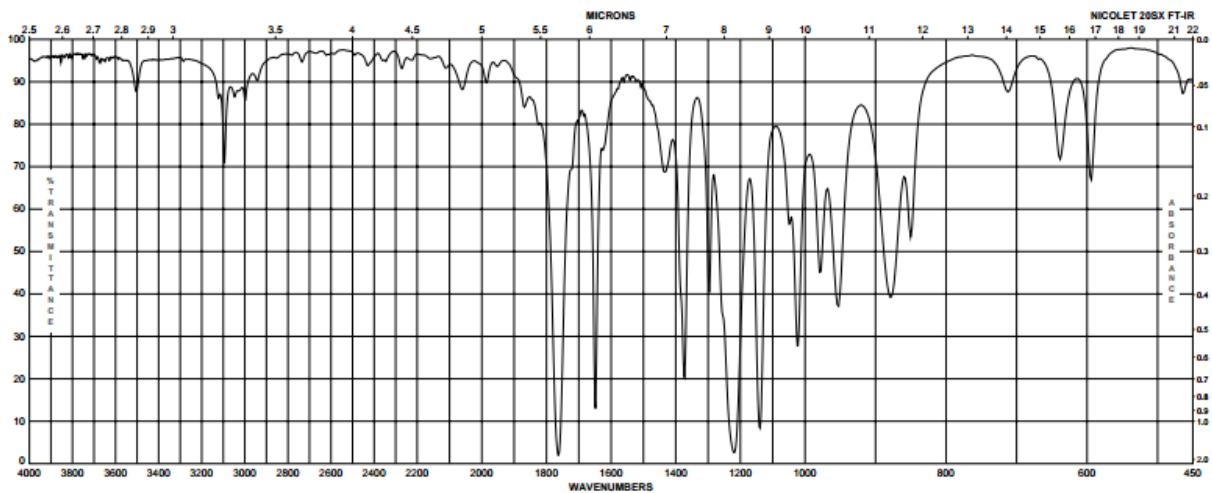


ethyl vinyl ether

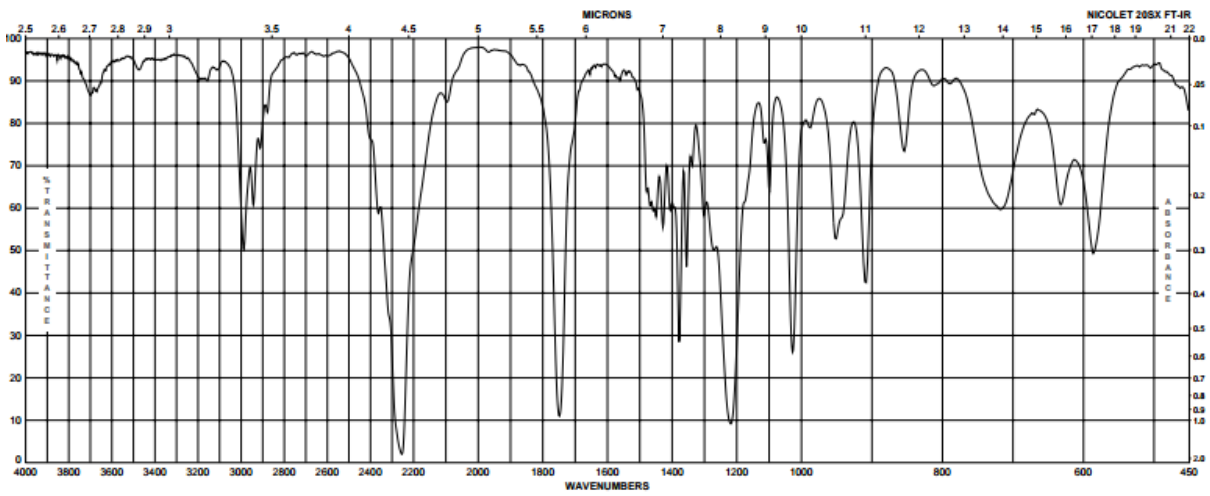


ethyl isocyanatoacetate

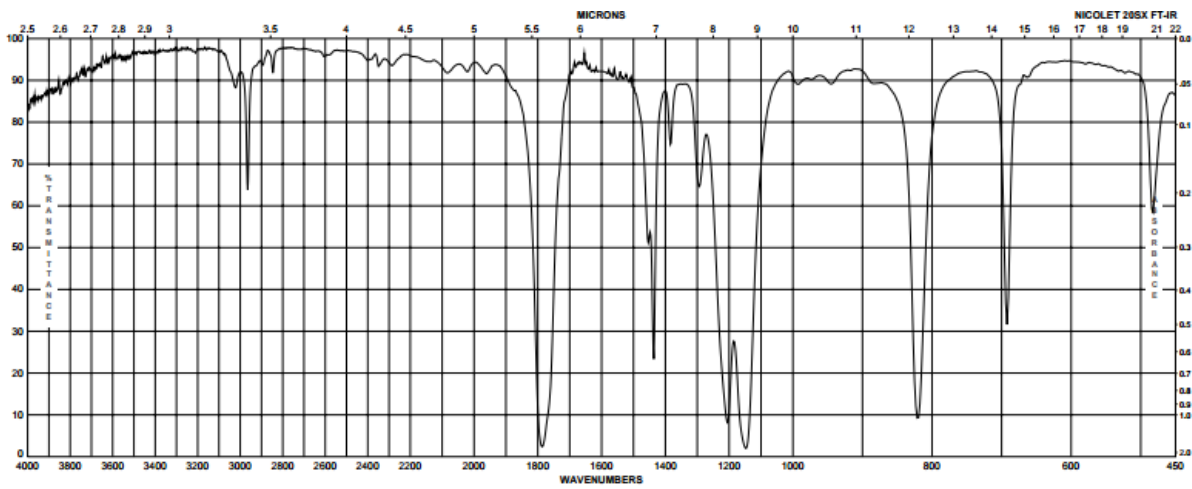
- (i) Spectrum 1 / spektrum 1: \_\_\_\_\_



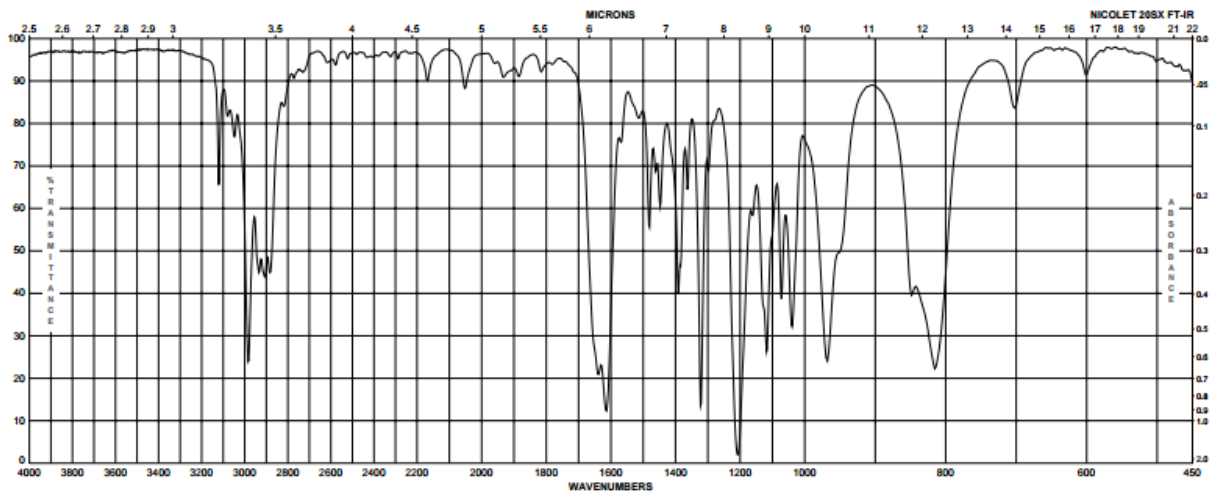
(ii) Spectrum 2/*spektrum 2*: \_\_\_\_\_



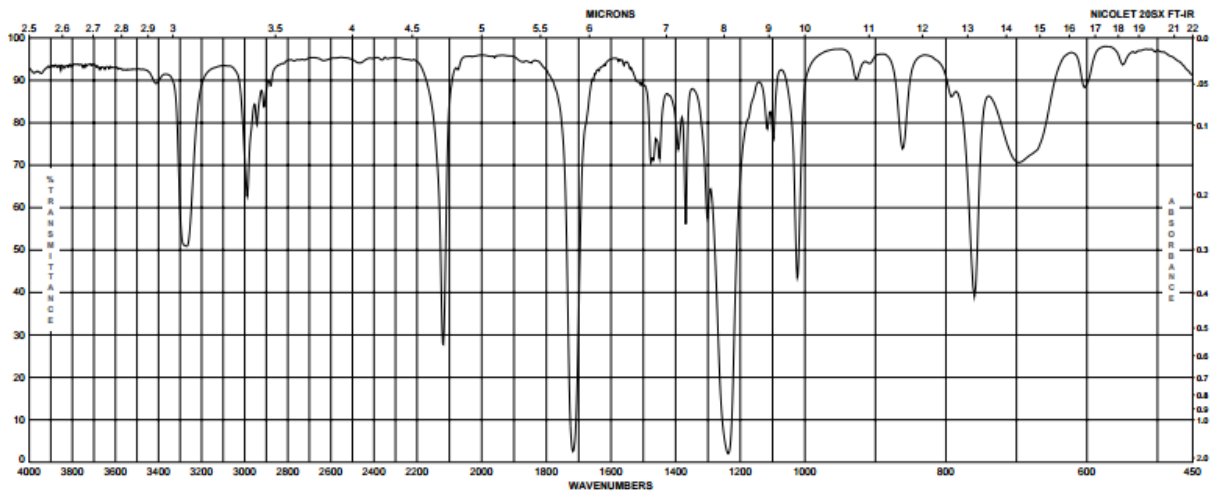
(iii) Spectrum 3/*spektrum 3*: \_\_\_\_\_



(iv) Spectrum 4/*spektrum 4*: \_\_\_\_\_



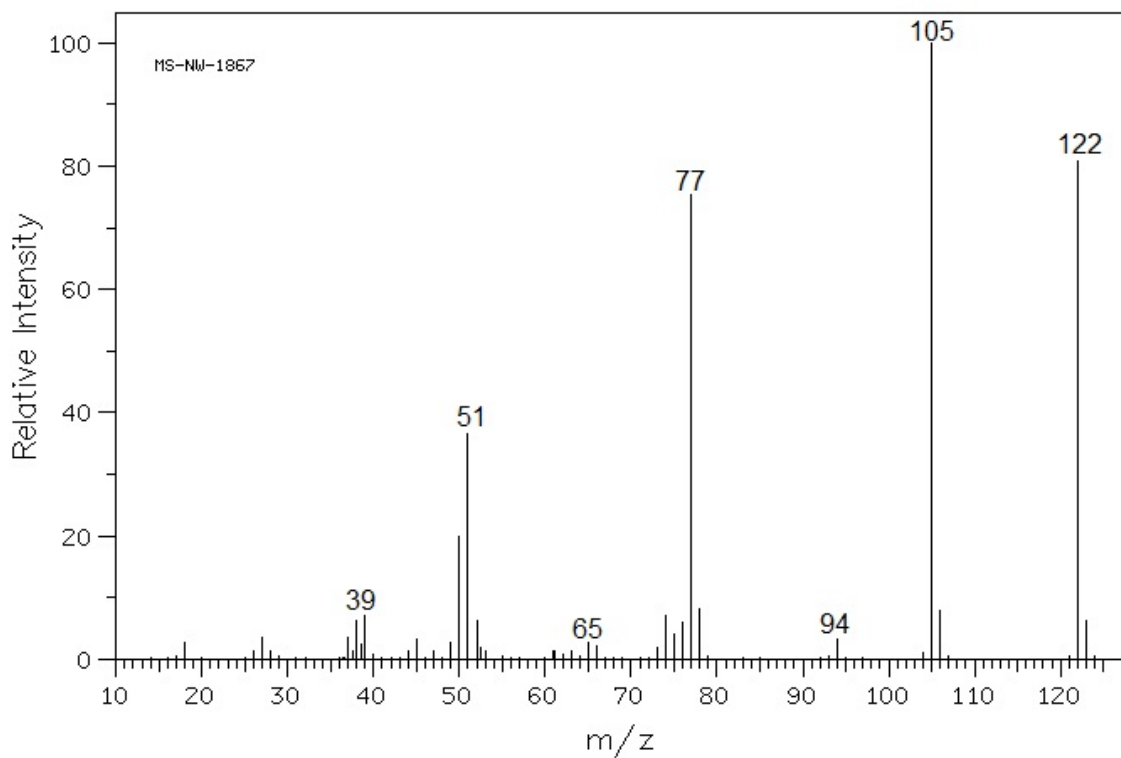
(v) Spectrum 5/*spektrum 5*: \_\_\_\_\_



(10 marks/*markah*)

2. (a) A benzoic acid,  $C_7H_6O_2$ , gives the following mass spectrum. Identify the major peaks. Associate the fragments responsible for the major peaks in the mass spectrum below.

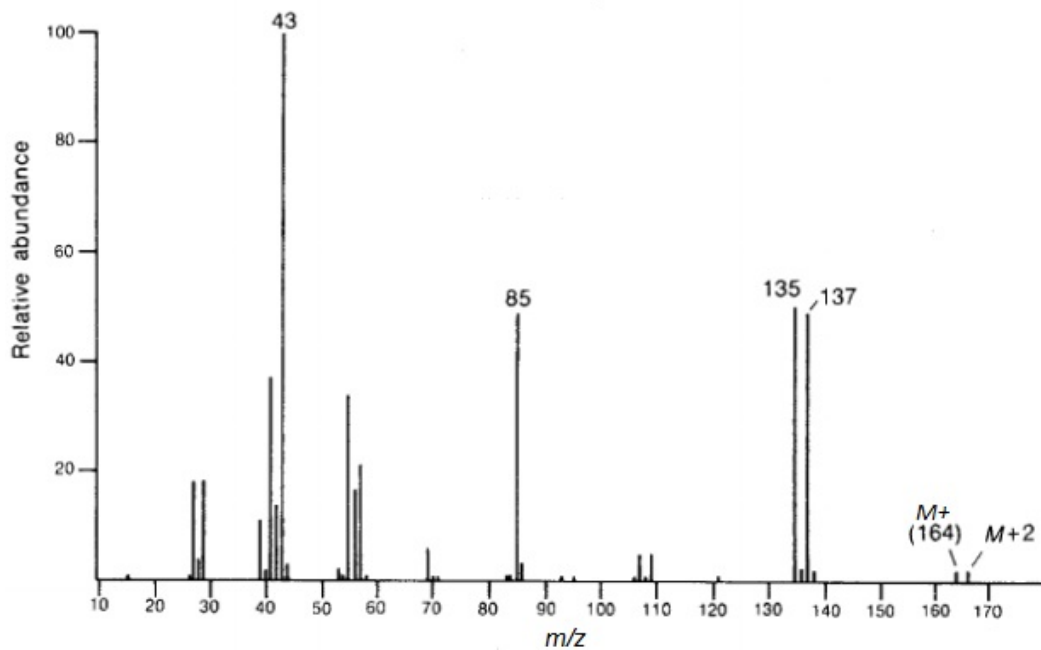
*Suatu asid benzoik,  $C_7H_6O_2$  memberikan spektrum jisim seperti berikut. Kenalpasti puncak-puncak utama. Hubungkan serpihan-serpihan yang menghasilkan puncak-puncak utama tersebut di dalam spektrum jisim di bawah.*



(5 marks/markah)

- 7 -

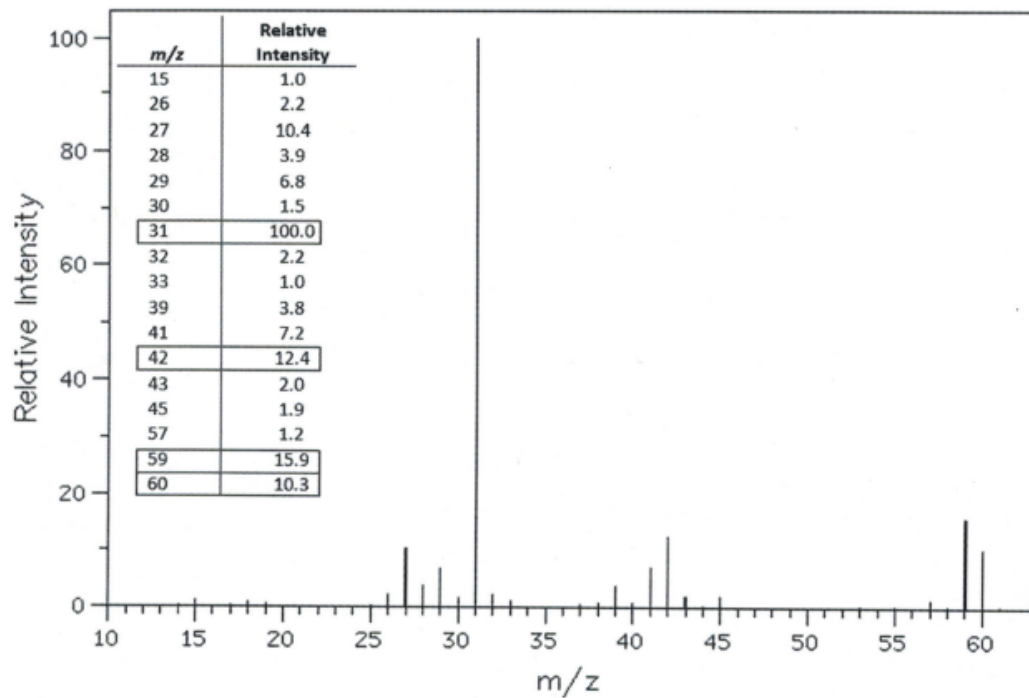
- (b) Provide a structure for the compound,  $C_6H_{13}Br$ , represented in the following mass spectrum. Draw the fragmentations that give rise to the  $m/z = 85$  and 135. *Berikan struktur untuk sebatian,  $C_6H_{13}Br$ , yang diwakili oleh spektrum jisim di bawah. Lukiskan penyerpihan yang menyumbang kepada  $m/z = 85$  dan 135.*



(5 marks/markah)

- (c) Using the mass spectrum of propan-1-ol shown below, answer the questions that follow about its fragmentation.

*Dengan menggunakan spektrum jisim bagi propan-1-ol seperti di bawah, jawab soalan berikut berkenaan dengan penyerpihannya.*



- (i) Draw a structure of the molecular ion formed and provide its  $m/z$  value.  
*Lukiskan struktur ion molekular yang terbentuk dan berikan nilai  $m/z$  nya.*
- (ii) Draw the structures of the fragments that produce the signals at  $m/z = 31, 59$  and  $42$ .  
*Lukiskan struktur-struktur serpihan yang menghasilkan isyarat pada  $m/z = 31, 59$  dan  $42$ .*
- (iii) Why does the peak at  $m/z = 15$  has a low relative intensity?  
*Mengapakah puncak pada  $m/z = 15$  mempunyai keamatan relatif yang rendah?*

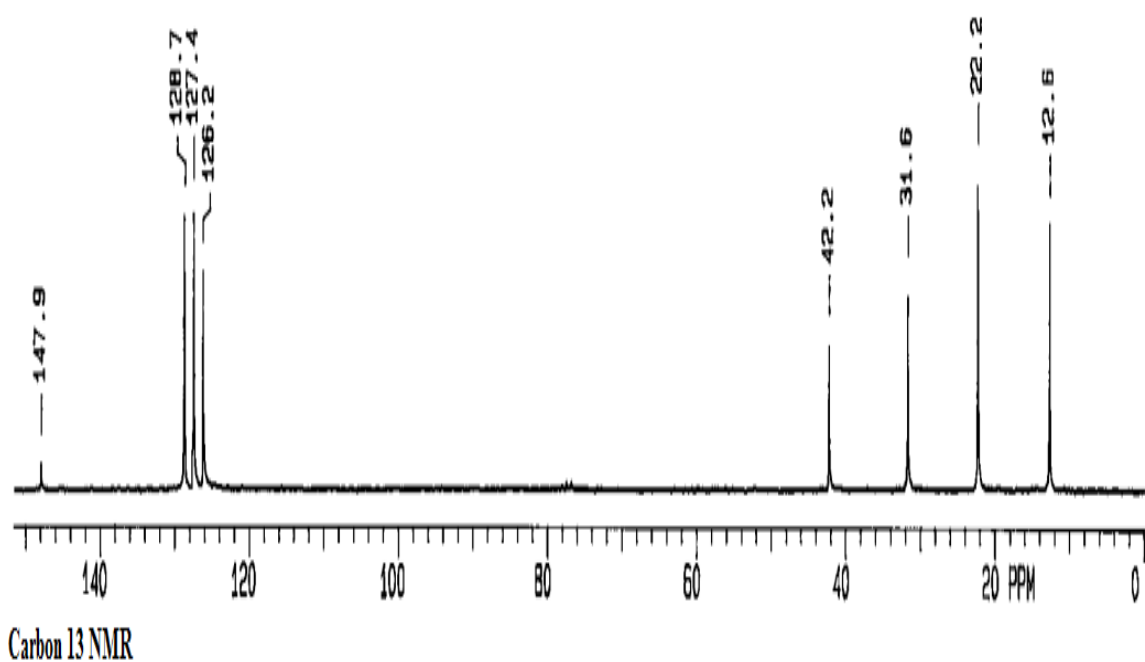
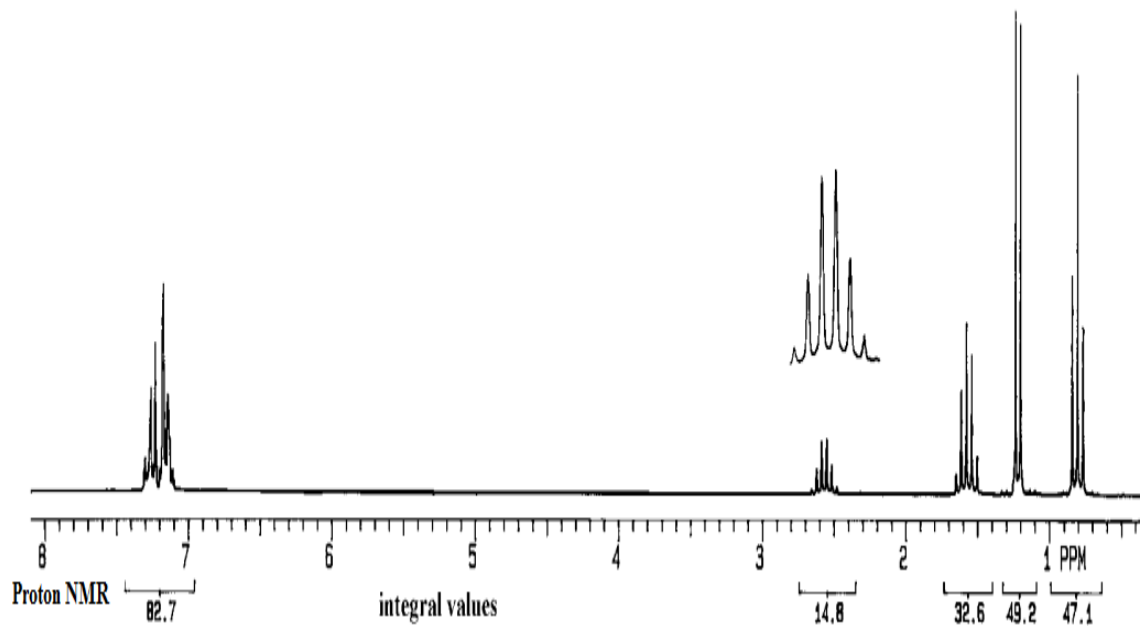
(10 marks/markah)



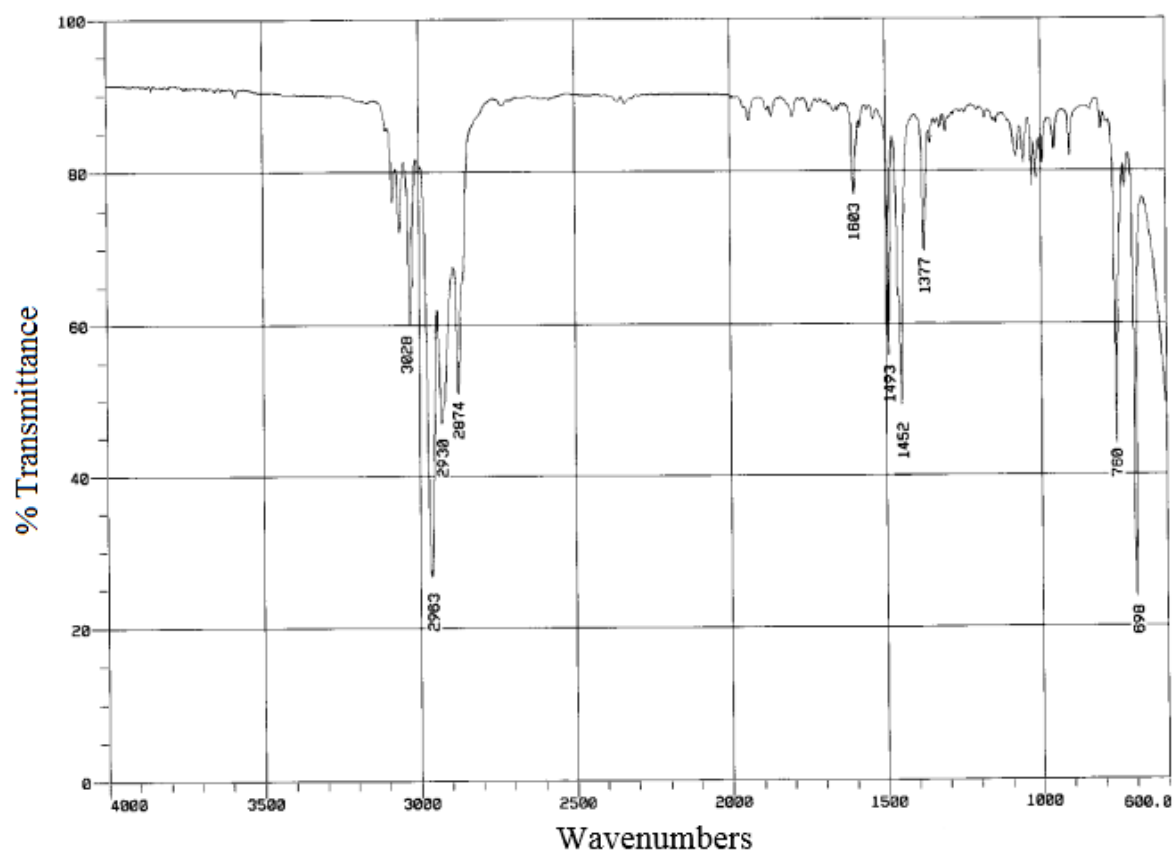
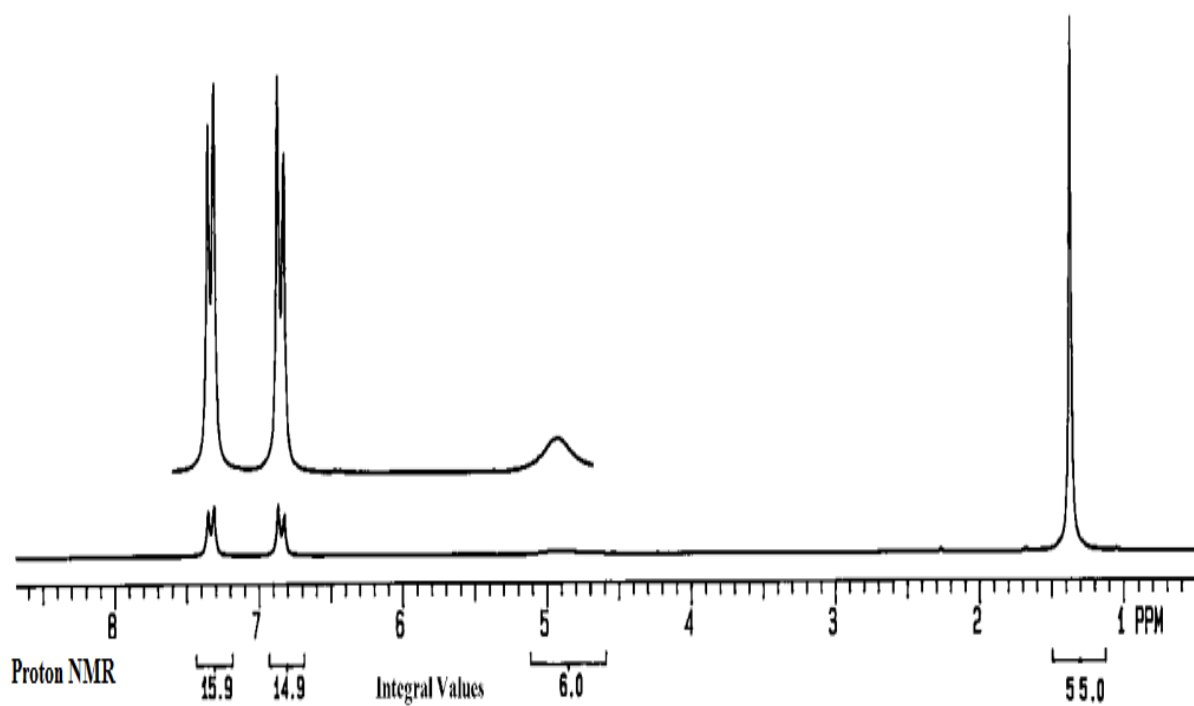
3. (a) Draw the structure of each of the following unknown compounds based on its molecular formula and its  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR and IR spectra. Explain your answer.

*Lukiskan struktur untuk setiap sebatian yang tidak diketahui di bawah berdasarkan formula molekul dan spektrum  $^1\text{H}$  NMR,  $^{13}\text{C}$  NMR serta IR masing-masing. Jelaskan jawapan anda.*

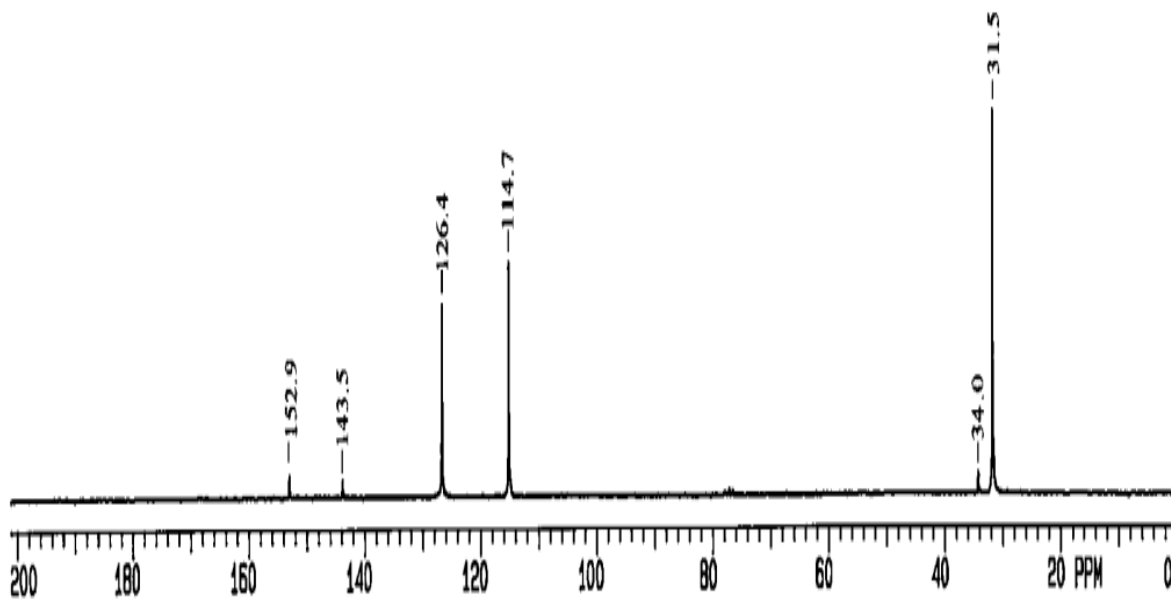
- (i)  $\text{C}_{10}\text{H}_{14}$



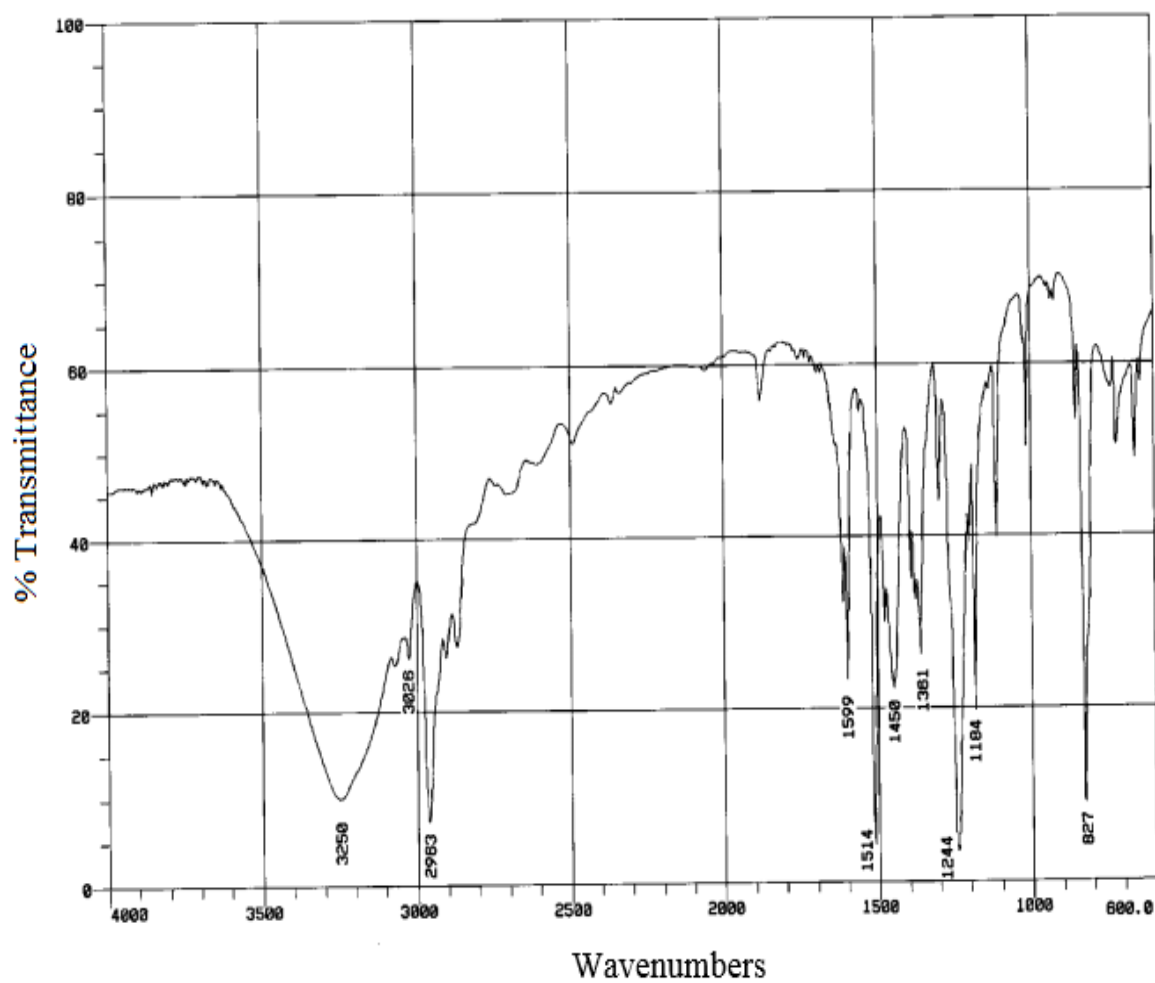
- 10 -

(ii)  $C_{10}H_{14}O$ 

..11/-



Carbon 13 NMR



(10 marks/markah)

- (b) Draw the  $^1\text{H-NMR}$  spectrum you would expect for the following compounds. Show clearly the splitting pattern and the integration values.

*Lukiskan spectrum  $^1\text{H-NMR}$  yang anda jangkakan untuk sebatian-sebatian di bawah. Tunjukkan dengan jelas pola pemecahan dan nilai integrasi.*



(10 marks/markah)

4. (a) Briefly explain the use of the following features in proton nuclear magnetic resonance (NMR) spectrum.

*Secara ringkas, terangkan penggunaan ciri-ciri yang berikut dalam spektrum resonans magnetik nuklear (NMR) proton.*

- (i) Peak multiplicity

*Kegandaan puncak*

- (ii) Chemical shift

*Anjakan kimia*

- (iii) Integral

*Kamiran*

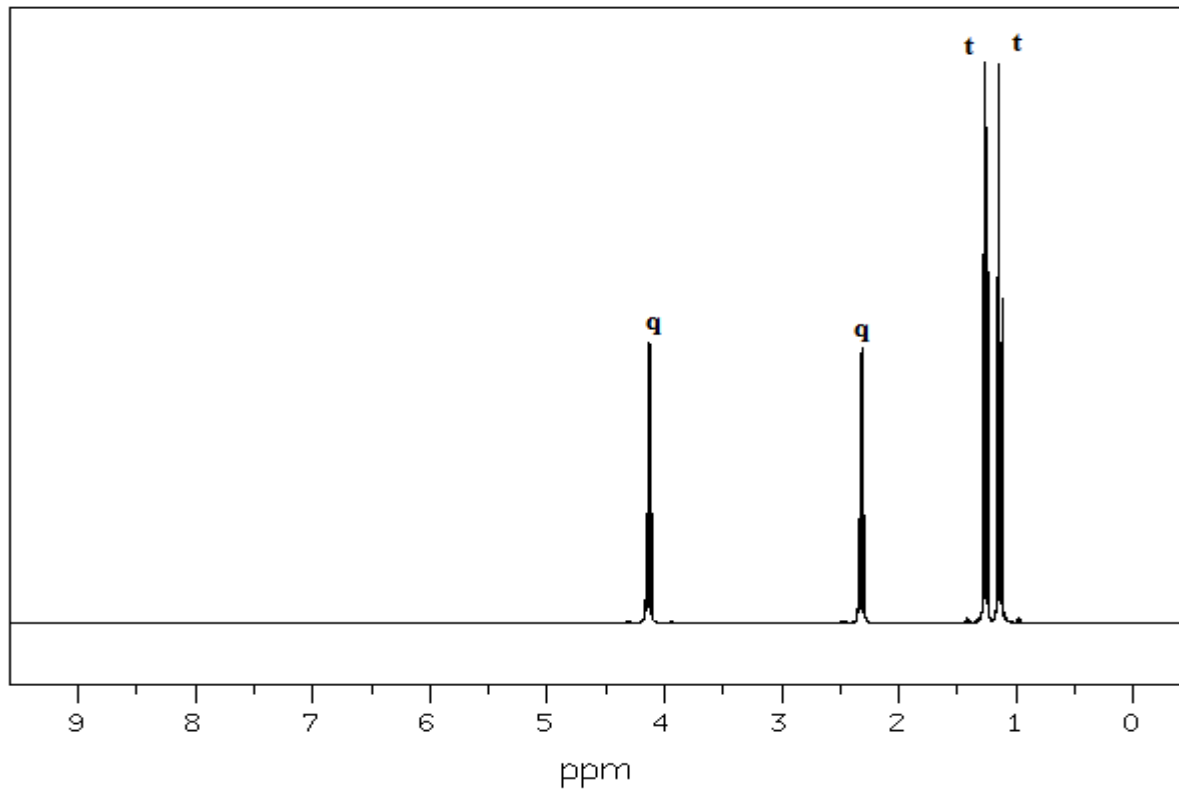
- (iv) Number of signals

*Bilangan isyarat*

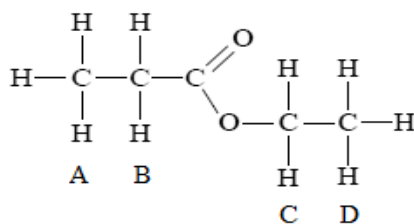
(4 marks/markah)

- (b) Below is a proton NMR spectra of ethyl propanoate obtained on a 400 MHz NMR spectrometer and chemical shift table.

*Di bawah adalah spektra proton NMR bagi etil propanoat yang diperoleh daripada 400 MHz NMR spektrometer dan jadual anjakan kimia.*



## Ethyl propanoate



Protons	Chemical Shift, $\delta$ (ppm)
A	1.140
D	1.259
B	2.319
C	4.132

- (i) With reasons indicate the most deshielded protons.

*Dengan memberikan alasan, nyatakan proton yang paling terdeshield.*

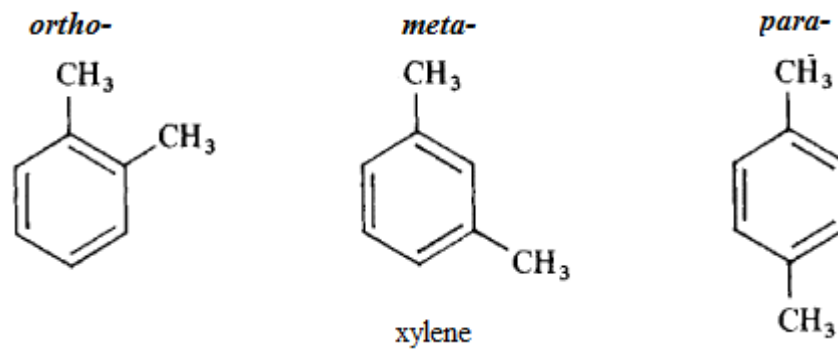
- (ii) The resonances for the A protons are split into 3 peaks. Explain the splitting and give the expected relative peak areas under the split peaks.

*Resonances bagi proton A berpecah kepada 3 puncak. Jelaskan pembelahan tersebut dan berikan jangkaan kawasan puncak relatif di bawah pembelahan puncak.*

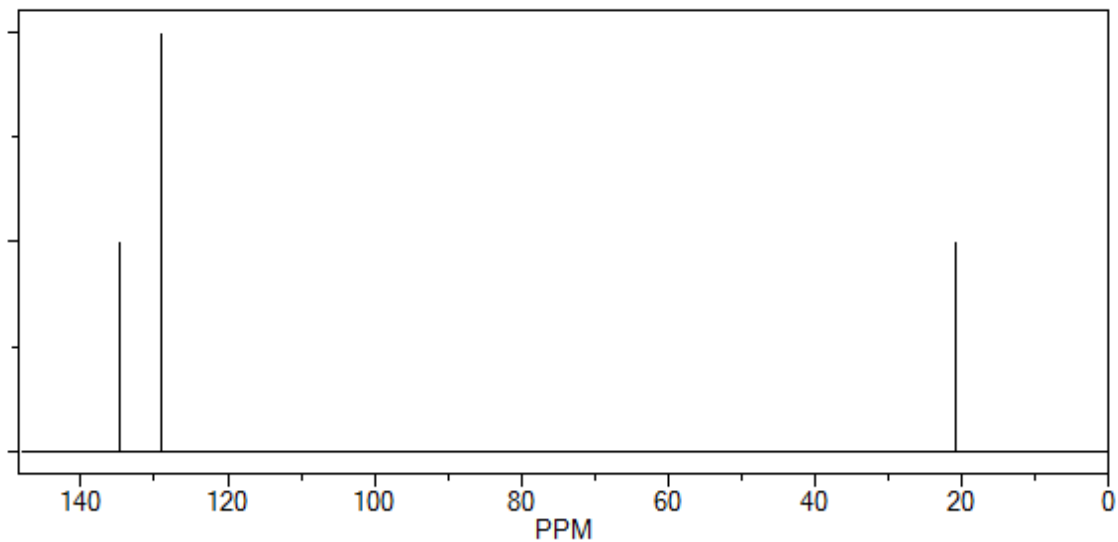
(8 marks/markah)

- (c) The three compounds shown below, *ortho*-, *meta*-, *para*-xylene have very different  $^{13}\text{C}$  NMR spectra. Match spectra A, B and C for each isomer.

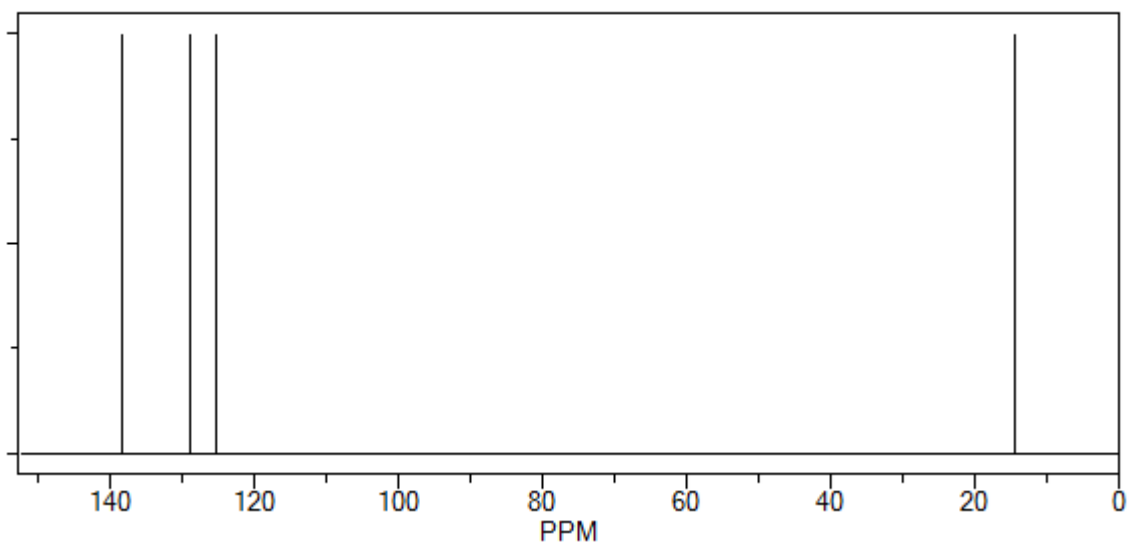
*Tiga sebatian yang ditunjukkan di bawah, ortho-, meta-, para-xylene mempunyai spektra  $^{13}\text{C}$  NMR yang berbeza. Padankan spektra A, B dan C untuk setiap isomer.*



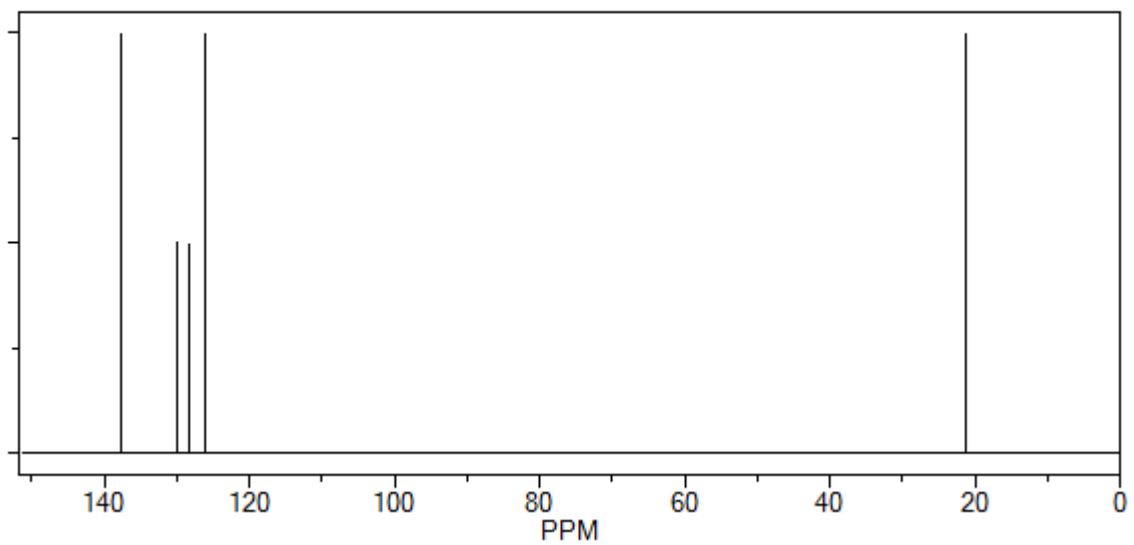
**Spectrum A:** .....



**Spectrum B:** .....



**Spectrum C:** .....

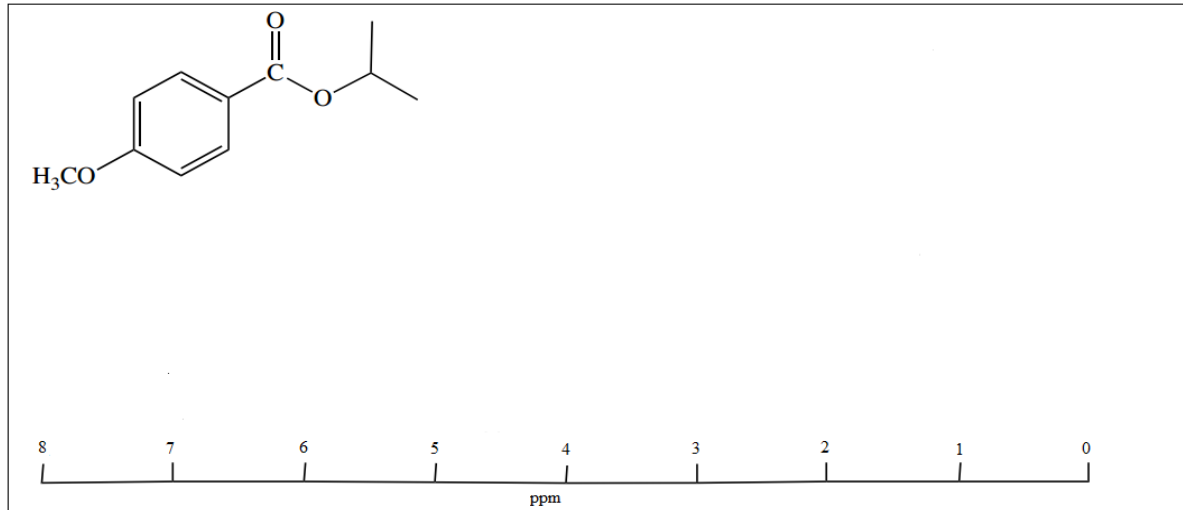


(3 marks/markah)



- (d) On the chart below, sketch the proton NMR spectrum that you would expect for the molecule shown.

*Pada carta di bawah, lakarkan spektrum NMR proton yang anda jangkakan untuk molekul yang ditunjukkan.*

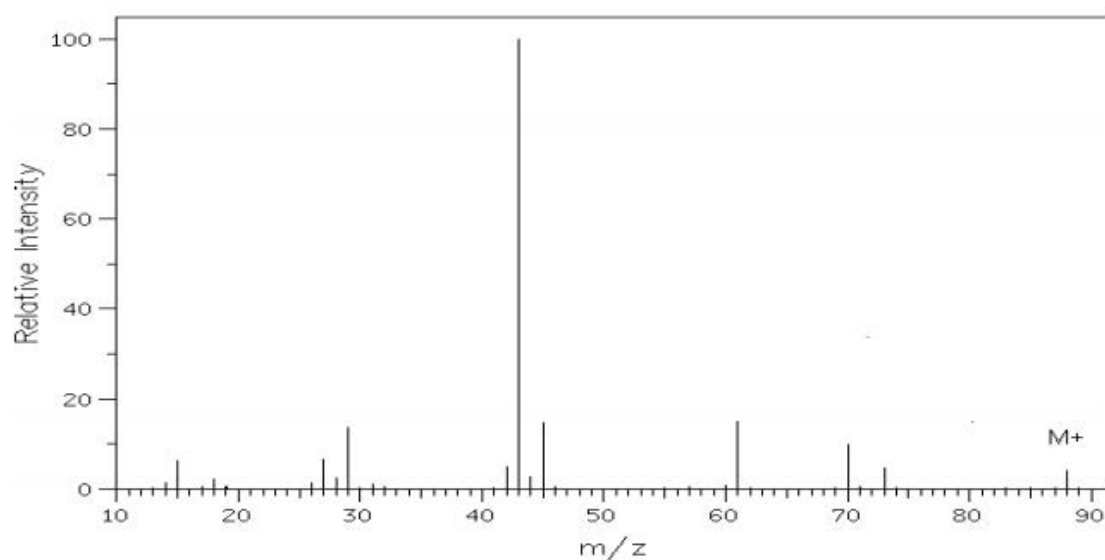


(5 marks/markah)

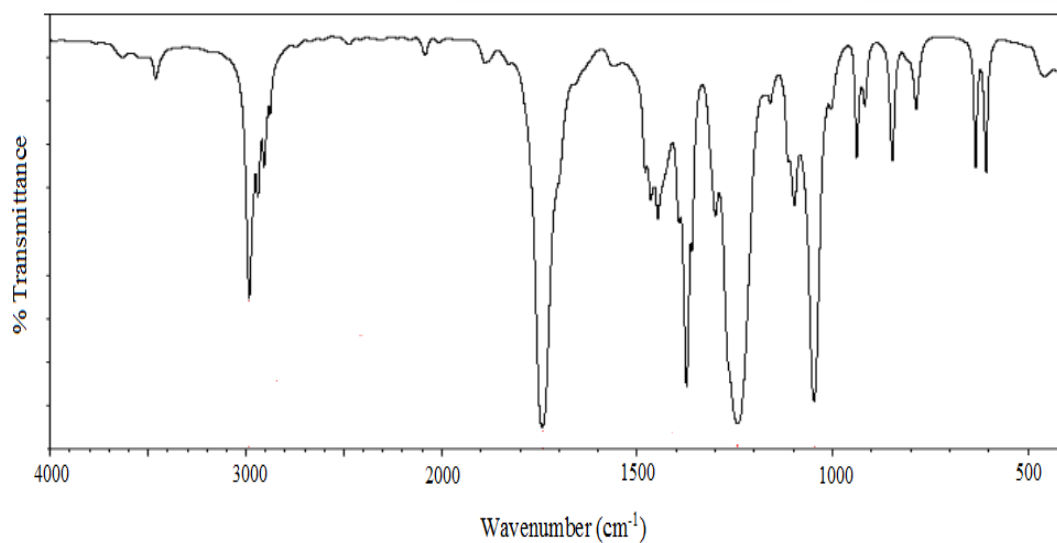
5. An unknown compound, **X** has the following mass, IR,  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra. Explain each spectrum individually and then consider them in relation to each other. Determine and draw the structure of compound **X**.

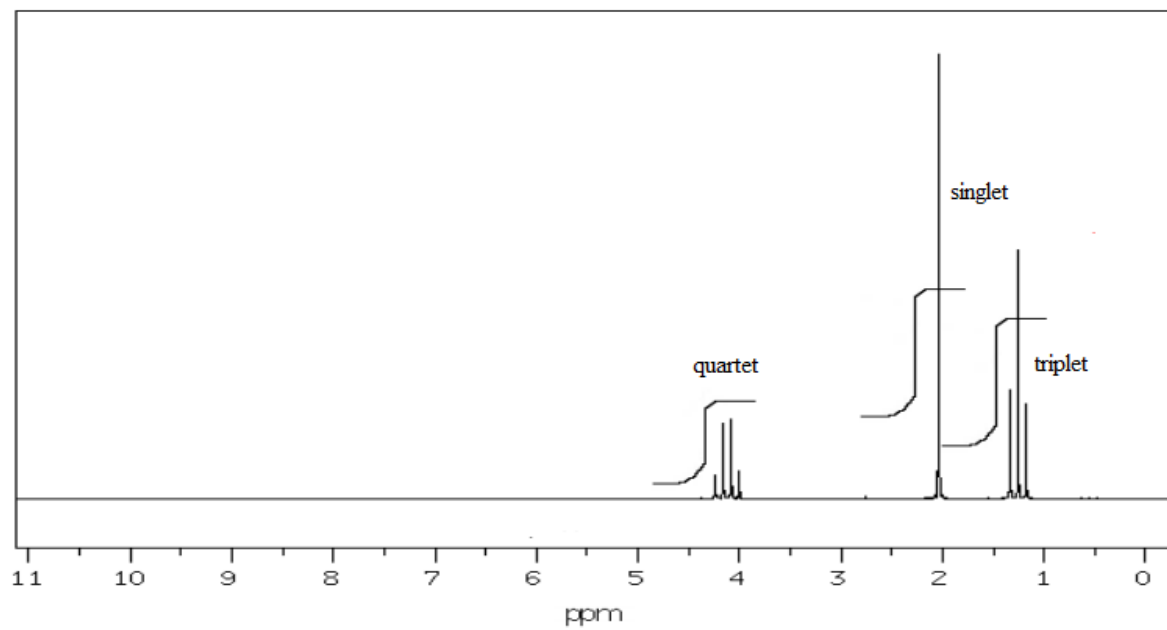
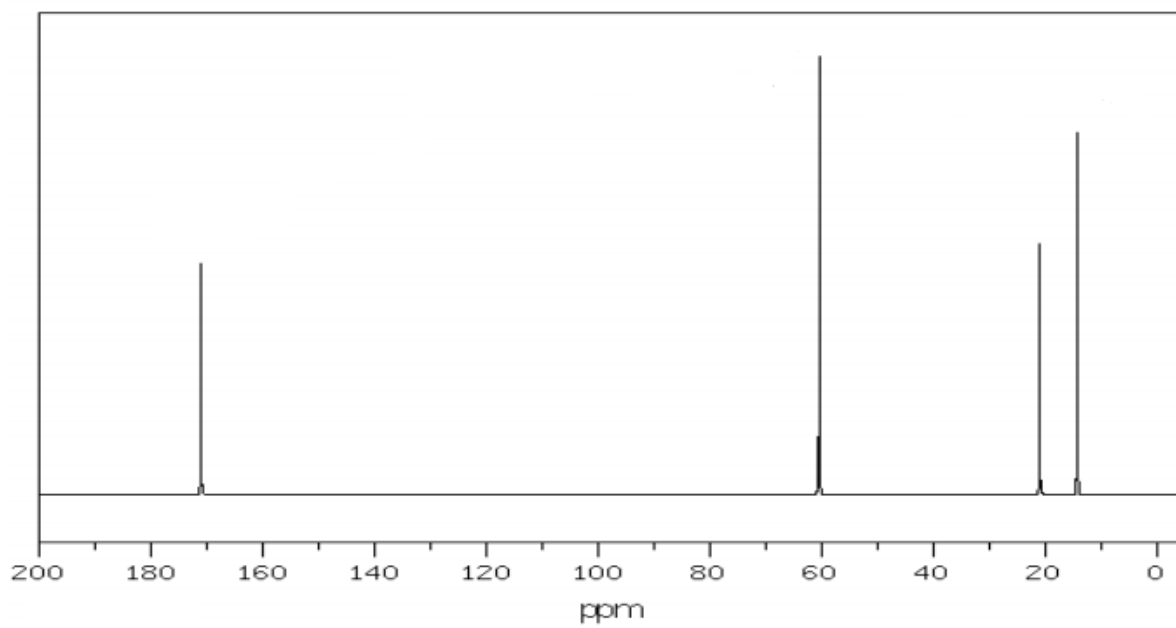
*Suatu sebatian yang tidak diketahui, X mempunyai data jisim, spectrum IR,  $^1\text{H}$  dan  $^{13}\text{C}$ -NMR seperti berikut. Jelaskan setiap spektrum secara berasingan dan kemudian pertimbangkan hubungannya antara satu sama lain. Tentukan dan lukis struktur sebatian X.*

### MS



### IR



**$^1\text{H}$ -NMR** **$^{13}\text{C}$ -NMR**

(20 marks/markah)

6. (a) Answer the questions below by referring to the  $C_{2h}$  character table.

*Jawab soalan di bawah dengan merujuk kepada jadual ciri  $C_{2h}$ .*

$C_{2h}$	E	$C_2$	i	$\sigma_h$
$A_g$	1	1	1	1
$B_g$	1	-1	1	-1
$A_u$	1	1	-1	-1
$B_u$	1	-1	-1	1

- (i) Taking the  $C_2$  axis as the z axis, and  $\sigma_h$  to be the xy plane, what do x, y and z represent in  $C_{2h}$  symmetry.

*Dengan mengambil kira paksi  $C_2$  sebagai paksi z, dan  $\sigma_h$  menjadi paksi xy, apakah yang diwakilkan oleh x, y dan z dalam simetri  $C_{2h}$ .*

- (ii) To what representations do the  $d_{xy}$ ,  $d_{xz}$  and  $d_{yz}$  orbitals belong in  $C_{2h}$  symmetry.

*Apakah yang diwakili oleh orbital  $d_{xy}$ ,  $d_{xz}$  dan  $d_{yz}$  dalam simetri  $C_{2h}$ .*

(6 marks/markah)

- (b) Find the irreducible representation for the following reducible ones.

*Dapatkan perwakilan tak terturunkan untuk data berikut.*

- (i)

$D_{3d}$	E	$2C_3$	$3C_2$	i	$2S_6$	$3\sigma_d$
	5	2	3	-1	2	1

- (ii)

$C_{6v}$	E	$2C_6$	$2C_3$	$C_2$	$3\sigma_v$	$3\sigma_d$
	4	-1	1	2	0	-2

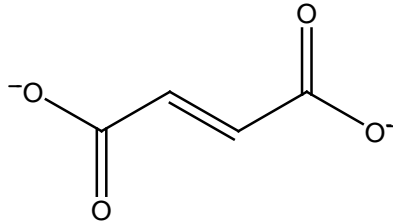
- (iii)

$T_d$	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
	8	2	0	2	2

(9 marks/markah)

- (c) Predict the IR and Raman vibrations in fumarate ion ( $C_{2h}$ ). Show your calculation.

*Ramalkan getaran IR dan Raman dalam ion fumarate ( $C_{2h}$ ). Tunjukkan pengiraan anda.*



fumarate ion

The ion lies in the  $xy$  plane. The  $C_2$  axis is the  $z$  axis.

*Ion tersebut terletak dalam satah  $xy$ . Paksi  $C_2$  adalah paksi  $z$ .*

(5 marks/markah)

IUPAC Periodic Table of the Elements

		Key:		atomic number		Symbol		name		standard atomic weight																													
1	<b>H</b> hydrogen [1.007, 1.009]	2	<b>He</b> helium 4.003	3	<b>Sc</b> scandium 44.96	4	<b>Ti</b> titanium 47.87	5	<b>V</b> vanadium 50.94	6	<b>Cr</b> chromium 51.99	7	<b>Mn</b> manganese 54.94	8	<b>Fe</b> iron 55.85	9	<b>Co</b> cobalt 58.93	10	<b>Ni</b> nickel 58.69	11	<b>Cu</b> copper 63.55	12	<b>Zn</b> zinc 65.38(2)	13	<b>B</b> boron [10.80, 10.83]	14	<b>C</b> carbon [12.00, 12.02]	15	<b>N</b> nitrogen [14.00, 14.01]	16	<b>O</b> oxygen [15.99, 16.00]	17	<b>F</b> fluorine 18.00	18	<b>Ne</b> neon 20.18				
3	<b>Li</b> lithium [6.938, 6.997]	4	<b>Be</b> beryllium 9.012	20	<b>Ca</b> calcium 40.08	21	<b>Sc</b> scandium 44.96	22	<b>Ti</b> titanium 47.87	23	<b>V</b> vanadium 50.94	24	<b>Cr</b> chromium 51.99	25	<b>Mn</b> manganese 54.94	26	<b>Fe</b> iron 55.85	27	<b>Co</b> cobalt 58.93	28	<b>Ni</b> nickel 58.69	29	<b>Cu</b> copper 63.55	30	<b>Zn</b> zinc 65.38(2)	31	<b>Ga</b> gallium 69.72	32	<b>Ge</b> germanium 72.63	33	<b>As</b> arsenic 74.92	34	<b>Se</b> selenium 78.97	35	<b>Br</b> bromine [79.90, 79.91]	36	<b>Kr</b> krypton 83.80		
11	<b>Na</b> sodium 22.99	12	<b>Mg</b> magnesium [24.30, 24.31]	37	<b>Rb</b> rubidium 85.47	38	<b>Sr</b> strontium 87.62	39	<b>Y</b> yttrium 88.91	40	<b>Zr</b> zirconium 91.22	41	<b>Nb</b> niobium 92.91	42	<b>Mo</b> molybdenum 95.96	43	<b>Tc</b> technetium 101.1	44	<b>Ru</b> ruthenium 101.07	45	<b>Rh</b> rhodium 102.9	46	<b>Pd</b> palladium 106.4	47	<b>Ag</b> silver 107.9	48	<b>Cd</b> cadmium 112.4	49	<b>In</b> indium 114.5	50	<b>Sn</b> tin 118.7	51	<b>Sb</b> antimony 121.8	52	<b>Te</b> tellurium 127.6	53	<b>I</b> iodine 126.9	54	<b>Xe</b> xenon 131.3
55	<b>Cs</b> caesium 132.9	56	<b>Ba</b> barium 137.3	57-71	lanthanoids	72	<b>Hf</b> hafnium 178.5	73	<b>Ta</b> tantalum 180.9	74	<b>W</b> tungsten 183.8	75	<b>Re</b> rhenium 186.2	76	<b>Os</b> osmium 190.2	77	<b>Ir</b> iridium 192.2	78	<b>Pt</b> platinum 195.1	79	<b>Au</b> gold 197.0	80	<b>Hg</b> mercury 200.6	81	<b>Tl</b> thallium [204.3, 204.4]	82	<b>Pb</b> lead 207.2	83	<b>Bi</b> bismuth 209.0	84	<b>Po</b> polonium	85	<b>At</b> astatine	86	<b>Rn</b> radon				
87	<b>Fr</b> francium	88	<b>Ra</b> radium	89-103	actinoids	104	<b>Rf</b> rutherfordium	105	<b>Db</b> dubnium	106	<b>Sg</b> seaborgium	107	<b>Bh</b> bohrium	108	<b>Hs</b> hassium	109	<b>Mt</b> meitnerium	110	<b>Ds</b> darmstadtium	111	<b>Rg</b> roentgenium	112	<b>Cn</b> copernicium	113	<b>Uut</b> ununium	114	<b>Ff</b> flerovium	115	<b>Uup</b> ununpentium	116	<b>Lv</b> livermorium	117	<b>Uus</b> ununseptium	118	<b>Uuo</b> ununoctium				



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PURE AND APPLIED CHEMISTRY

57	<b>La</b> lanthanum 138.9	58	<b>Ce</b> cerium 140.1	59	<b>Pr</b> praseodymium 140.9	60	<b>Nd</b> neodymium 144.2	61	<b>Pm</b> promethium	62	<b>Sm</b> samarium 150.4	63	<b>Eu</b> europium 152.0	64	<b>Gd</b> gadolinium 157.3	65	<b>Tb</b> terbium 158.9	66	<b>Dy</b> dysprosium 162.5	67	<b>Ho</b> holmium 164.9	68	<b>Er</b> erbium 167.3	69	<b>Tm</b> thulium 168.9	70	<b>Yb</b> ytterbium 173.0	71	<b>Lu</b> lutetium 175.0
89	<b>Ac</b> actinium 227.0	90	<b>Th</b> thorium 232.0	91	<b>Pa</b> protactinium 231.0	92	<b>U</b> uranium 238.0	93	<b>Np</b> neptunium	94	<b>Pu</b> plutonium	95	<b>Am</b> americium	96	<b>Cm</b> curium	97	<b>Bk</b> berkelium	98	<b>Cf</b> californium	99	<b>Es</b> einsteinium	100	<b>Fm</b> fermium	101	<b>Md</b> mendelevium	102	<b>No</b> nobelium	103	<b>Lr</b> lawrencium

For notes and updates to this table, see www.iupac.org. This version is dated 8 January 2016.  
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## Supplementary data

Rules of Diene Absorption	
Base value for heteroannular diene	214
Base value for homoannular diene	253
Increments for	
Double bond extending conjugation	+30
Alkyl substituent or ring residue	+5
Exocyclic double bond	+5
Polar groupings:	
OAc	+0
OAlk	+6
SAlk	+30
Cl, Br	+5
N(Alk) <sub>2</sub>	+60
Solvent correction	+0
	$\lambda_{calc} = Total$

**Reducing Formula**

$$a_i = 1/h \sum X_R^s X_i^s N^s$$

$h$  ; total number of operations in certain point group.

$X_R^s$  ; Character ( $X$ ) for reducible representation.

$X_i^s$  ; Character ( $X$ ) for reducible representation (from the character Table)

$N^s$  ; Number of symmetry operation for each type or class of operation.

**Contribution for the Character,  $\chi(R)$ , for each unshifted atom in  $\Gamma_{3N}$**

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R	$\chi(R)$
E	+3
i	-3
$\sigma$	+1
$C_2$	-1
$C_3^1, C_3^2$	0
$C_4^1, C_4^3$	+1
$C_6^1, C_6^5$	+2
$S_3^1, S_3^5$	-2
$S_4^1, S_4^3$	-1
$S_6^1, S_6^5$	0



## Notations of the Character Table

a	b		
f	c	d	e

a. Schoenflies symbols for point group

b. lists the symmetry operations (by classes) for that group

c. lists all the characters, for all irreducible representations, of each class of each operation

d. shows the irreducible representations for which the six vectors,  $T_x, T_y, T_z, R_x, R_y, R_z$ , provide the bases

e. shows the functions which are binary combinations of  $x, y, z$  (e.g.  $xy, z^2$ ) provide bases for certain irreducible representations

f. lists conventional symbols for the irreducible representations called *Mulliken symbols*. All one-dimensional irreducible rep. are labelled as A or B, all two-dimensional as E, all three-dimensional as T (in certain texts it is given the label F), four-dimensional as G and five-dimensional as H.

In addition to the letter, most Mulliken symbols possess certain subscripts and/or superscripts. For two- and higher-dimensional irreducible representations they can be regarded as labels. For one-dimensional representations, they have the following specifications.

A : One-dimensional irreducible rep. if it is symmetry about  $C_n$  axis, i.e. ( $\chi = +1$ )

B : " " " antisymm. " ( $\chi = -1$ )

Sub.<sub>1</sub> : Irr. Rep is symmetry with respect to  $C_2 \perp C_n$  (if no  $C_2$ ), then  
Irr. Rep. Is symmetry with respect to  $\sigma_v$

Sub.<sub>2</sub> : Irr. Rep is antisymmetry under conditions as those in Sub.<sub>1</sub> of above.

Sub.<sub>g</sub> : (gerade) irr. rep. are symm. With respect to inversion at an i

Sub.<sub>u</sub> : (ungerade) irr. rep. are antisymm. with respect to an i

' : irr. Rep are symm with respect to reflection in a  $\sigma_h$

" : irr. Rep. Are antisymm with respect to reflection in a  $\sigma_h$

The  $C_{nh}$  Groups

$C_{2h}$	$C_2$	$C_s$	$C_i$	$C_{3h}$	$C_3$	$C_s$
$A_g$	A	A'	$A_g$	A'	A	A'
$B_g$	B	A''	$A_g$	E'	E	2A'
$A_u$	A	A''	$A_u$	A''	A	A''
$B_u$	B	A'	$A_u$	E''	E	2A''
$C_{4h}$	$C_4$	$S_4$	$C_{2h}$	$C_2$	$C_s$	$C_i$
$A_g$	A	A	$A_g$	A	A'	$A_g$
$B_g$	B	B	$A_g$	A	A'	$A_g$
$E_g$	E	E	2 $B_g$	2A''	2A'	2 $A_g$
$A_u$	A	B	$A_u$	A''	A	$A_u$
$B_u$	B	A	$A_u$	A''	A	$A_u$
$E_u$	E	E	2 $B_u$	2A'	2A'	2 $A_u$
				$C_{5h}$	$C_5$	$C_s$
				A'	A	A'
				E <sub>1</sub> '	E <sub>1</sub>	2A'
				E <sub>2</sub> '	E <sub>2</sub>	2A'
				A''	A	A''
				E <sub>1</sub> ''	E <sub>1</sub>	2A''
				E <sub>2</sub> ''	E <sub>2</sub>	2A''

The  $C_{nv}$  Groups

$C_{2v}$	$C_2$	$C_s$	$C_3$	$C_{3v}$	$C_3$	$C_s$
$A_1$	A	$A'$	$A'$	$A_1$	A	$A'$
$A_2$	A	$A''$	$A''$	$A_2$	A	$A''$
$B_1$	B	$A'$	$A''$	E	E	$A' + A''$
$B_2$	B	$A''$	$A'$			

$C_{4v}$	$C_4$	$C_{2v}$	$C_2$	$C_s$	$C_3$	$\sigma_v$	$\sigma_d$
$A_1$	A	$A_1$	A	$A'$	$A'$	$A'$	$A'$
$A_2$	A	$A_2$	A	$A''$	$A''$	$A''$	$A''$
$B_1$	B	$A_1$	A	$A'$	$A'$	$A'$	$A''$
$B_2$	B	$A_2$	A	$A''$	$A''$	$A''$	$A'$
E	E	$B_1 + B_2$	$B_1 + B_2$	$A' + A''$	$A' + A''$	$A' + A''$	$A' + A''$

$C_{5v}$	$C_5$	$C_3$	$C_6$	$C_{3v}$	$C_{2v}$	$C_3$	$C_2$	$C_3$	$\sigma_v$	$\sigma_d$
$A_1$	A	$A'$	A	$A_1$	$A_1$	A	A	A	$A'$	$A'$
$A_2$	A	$A''$	A	$A_2$	$A_2$	A	A	A	$A''$	$A''$
$E_1$	$E_1$	$A' + A''$	B	$A_1$	$B_1$	A	B	A	$A'$	$A''$
$E_2$	$E_2$	$A' + A''$	B	$A_2$	$B_2$	A	B	A	$A''$	$A'$
			$E_1$	E	$B_1 + B_2$	E	$2B$	E	$A' + A''$	$A' + A''$
			$E_2$	E	$A_1 + A_2$	E	$2A$	E	$A' + A''$	$A' + A''$

The  $D_{nd}$  Groups

$D_{2d}$	$C_2 \rightarrow C_2(z)$			$C_2$	$C_2'$	$C_s$
	$S_4$	$D_2$	$C_{2v}$	$C_2$	$C_2$	
$A_1$	A	A	$A_1$	A	A	$A'$
$A_2$	A	$B_1$	$A_2$	A	B	$A''$
$B_1$	B	A	$A_2$	A	A	$A''$
$B_2$	B	$B_1$	$A_1$	A	B	$A'$
E	E	$B_2 + B_3$	$B_1 + B_2$	2B	$A + B$	$A' + A''$

$D_{3d}$	$D_3$	$C_{3v}$	$S_6$	$C_3$	$C_{2h}$	$C_2$	$C_2$	$C_i$
	$A_{1g}$	$A_1$	$A_1$	$A_g$	A	$A_g$	A	$A'$
$A_{2g}$	$A_2$	$A_2$	$A_g$	A	$B_g$	B	$A''$	$A_g$
$E_g$	E	E	$E_g$	E	$A_g + B_g$	$A + B$	$A' + A''$	$2A_g$
$A_{1u}$	$A_1$	$A_2$	$A_u$	A	$A_u$	A	$A''$	$A_u$
$A_{2u}$	$A_2$	$A_1$	$A_u$	A	$B_u$	B	$A'$	$A_u$
$E_u$	E	E	$E_u$	E	$A_u + B_u$	$A + B$	$A' + A''$	$2A_u$

$D_{4d}$	$D_4$	$C_{4v}$	$S_8$	$C_4$	$C_{2v}$	$C_2$	$C_2'$	$C_s$
						$C_2$	$C_2$	
$A_1$	$A_1$	$A_1$	A	A	$A_1$	A	A	$A'$
$A_2$	$A_2$	$A_2$	A	A	$A_2$	A	B	$A''$
$B_1$	$A_1$	$A_2$	B	A	$A_2$	A	A	$A''$
$B_2$	$A_2$	$A_1$	B	A	$A_1$	A	B	$A'$
$E_1$	E	E	$E_1$	E	$B_1 + B_2$	2B	$A + B$	$A' + A''$
$E_2$	$B_1 + B_2$	$B_1 + B_2$	$E_2$	2B	$A_1 + A_2$	2A	$A + B$	$A' + A''$
$E_3$	E	E	$E_3$	E	$B_1 + B_2$	2B	$A + B$	$A' + A''$

$D_{5d}$	$D_5$	$C_{5v}$	$C_5$	$C_2$	$C_s$	$C_i$
	$A_{1g}$	$A_1$	$A_1$	A	A	$A'$
$A_{2g}$	$A_2$	$A_2$	A	B	$A''$	$A_g$
$E_{1g}$	$E_1$	$E_1$	$E_1$	$A + B$	$A' + A''$	$2A_g$
$E_{2g}$	$E_2$	$E_2$	$E_2$	$A + B$	$A' + A''$	$2A_g$
$A_{1u}$	$A_1$	$A_2$	A	A	$A''$	$A_u$
$A_{2u}$	$A_2$	$A_1$	A	B	$A'$	$A_u$
$E_{1u}$	$E_1$	$E_1$	$E_1$	$A + B$	$A' + A''$	$2A_u$
$E_{2u}$	$E_2$	$E_2$	$E_2$	$A + B$	$A' + A''$	$2A_u$

*The T<sub>d</sub> Groups*

$T_d$	$D_{2d}$	$C_{3v}$	$S_4$	$D_2$	$C_{2v}$	$C_3$	$C_2$	$C_s$
$A_1$	$A_1$	$A_1$	$A$	$A$	$A_1$	$A$	$A$	$A'$
$A_2$	$B_1$	$A_2$	$B$	$A$	$A_2$	$A$	$A$	$A''$
$E$	$A_1 + B_1$	$E$	$A + B$	$2A$	$A_1 + A_2$	$E$	$2A$	$A' + A''$
$T_1$	$A_2 + E$	$A_2 + E$	$A + E$	$B_1 + B_2 + B_3$	$A_2 + B_1 + B_2$	$A + E$	$A + 2B$	$A' + 2A''$
$T_2$	$B_2 + E$	$A_1 + E$	$B + E$	$B_1 + B_2 + B_3$	$A_1 + B_1 + B_2$	$A + E$	$A + 2B$	$2A' + A''$